

Comment on “New Scaling of Child-Langmuir Law in the Quantum Regime”

Debabrata Biswas

Theoretical Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085, INDIA

In their letter on the quantum Child-Langmuir law, Ang et al [1] include exchange correlation effects within the Kohn-Sham density functional theory (DFT) [2] and explore numerically the maximum transmitted current (J_{max}) in nanogaps. We show here that the calculations are in error as the exchange-correlation component of the chemical potential has been ignored while fixing the boundary conditions for the Hartree potential.

The analysis in [1] is based on solving the time-independent Schrodinger equation $-d^2\psi/dx^2 + V_{eff}\psi = E\psi$ with an effective potential energy, $V_{eff} = -eV + V_{xc} \times E_H$, where $E_H = e^2/(4\pi\epsilon_0 a_0)$ is the Hartree energy, a_0 the Bohr radius, $V_{xc} = \epsilon_{xc} - (r_s/3)d\epsilon_{xc}/dr_s$, $r_s = [3/(4\pi n)]^{1/3}$ is the Wigner-Seitz radius, n the electron number density and e the magnitude of the electronic charge. In the above, ϵ_{xc} is the exchange-correlation energy density within the local density approximation, and V is the Hartree potential satisfying the Poisson equation $d^2V/dx^2 = en(x)/\epsilon_0 = e|\psi(x)|^2/\epsilon_0$ with boundary conditions $V(0) = 0$ and $V(D) = V_g$ where V_g is the gap voltage difference and D the gap size. These equations are solved in a nanogap with the wavefunction ψ and its derivative matched at the collector boundary under certain assumptions (Ref. [3] addresses one of these).

We first note that the applied voltage difference, $V_g = -(\mu_C - \mu_E)/e$ where μ_C and μ_E refer respectively to the chemical potential at the collector and injection planes. For convenience, we consider the reference as $\mu_E = -eV(0) + V_{xc}(0) \times E_H = 0$ so that $E = 0$ refers to injection from the Fermi level. Thus $V(0) = V_{xc}(0) \times E_H/e$. It follows that the chemical potential at the collector is $-eV(D) + V_{xc}(D) \times E_H = -eV_g$. Thus $V(D) = V_g + V_{xc}(D) \times E_H/e$. In writing the above, we have implicitly assumed continuity of the chemical potential at the interfaces under steady-state conditions. Note that when exchange-correlation is neglected altogether, the boundary conditions for V are $V(0) = 0$ and $V(D) = V_g$ respectively as assumed in [1].

When V_{xc} is substantial, and the boundary conditions chosen are $V(D) = V_g$ and $V(0) = 0$, the results can be unphysical. As an example, consider the case $D = 1\text{nm}$, $V_g = 0.1\text{V}$ and $E = 0$. Using the formalism of Ref. [1], J_{max} turns out to be $J_{max} \simeq 278J_{CL}$ where J_{CL} is the classical Child-Langmuir current density. The corresponding effective potential energy is shown in Fig. 1. Note that V_{eff} is negative everywhere. The injection energy E has clearly no relation to the effective potential at either end of the nanogap.

The corrected boundary conditions for V lead to

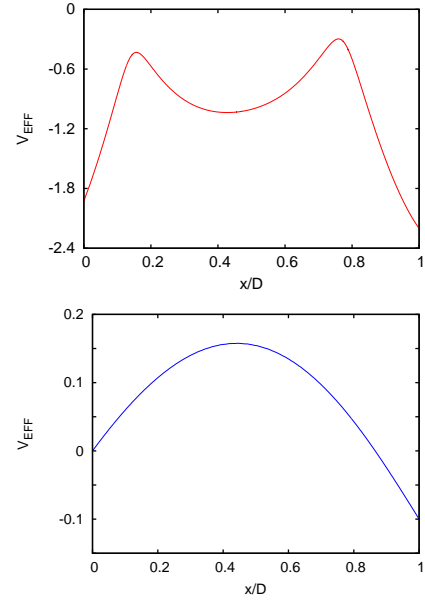


FIG. 1: The effective potential energy $V_{eff} = -eV + E_H \times V_{xc}$ for $D = 1\text{nm}$, $V_g = 0.1\text{V}$ (**top**) $V(0) = 0$, $V(D) = V_g$ and $J_{max} \simeq 278J_{CL}$ (**bottom**) $V(0) = V_{xc}(0) \times E_H/e$, $V(D) = V_g + V_{xc}(D) \times E_H/e$ and $J_{max} \simeq 3.4J_{CL}$. The boundary conditions for ψ are the same as in Ref. [1] in both cases.

$J_{max} \simeq 3.4J_{CL}$. The corresponding effective potential is shown in Fig. 1 (bottom). The error in determining the quantum Child-Langmuir law is therefore substantial.

In regimes where V_{xc} is negligible (large V_g or D), $V(D) = V_g$ and $V(0) = 0$ are approximately the correct boundary conditions within the formalism of Ref. [1] as we have verified for $D = 50\text{nm}$, $V_g = 50\text{V}$ and $E = 0$.

Finally, we note that the error in boundary conditions for V persists in subsequent publications by the authors of Ref. [1]. Results incorporating the rectified boundary conditions for V and improved boundary conditions for ψ will be published in a separate communication.

The author acknowledges fruitful discussions with Dr. Raghwendra Kumar and Dr. Biplab Ghosh.

-
- [1] L. K. Ang, T. J. T. Kwan, and Y. Y. Lau, Phys. Rev. Lett. **91**, 208303 (2003).
 - [2] W. Kohn and L. J. Sham, Phys. Rev. **140** A1133 (1965).
 - [3] D. Biswas and R. Kumar, Eur. Phys. J. B **85** (2012) 189.